**Advances in computational and experimental studies of solids**

**Cosener’s House, Abingdon**

**Monday 10th April 2017**

**13:00 Registration**

**13:50 Welcome and Introduction: Rob Jackson, Richard Catlow**

***Session 1: Energy Materials (Chair: Alan Chadwick)***

14:00 S Islam: Insights into Energy Materials – Batteries Included

14:20 J M Thomas: A selection of Vignettes

14:50 P Ngoepe: Simulated synthesis, characterisation and performance of nanoarchitectured energy storage materials for advanced batteries

15:10 L Briquet: Computational modelling applied to energy conversion materials

15:30 R Grimes: Fission gas in fuel: 40 years of simulations. Is the end in sight?

15:50 D Scanlon: Designing the next generation of oxide thermoelectrics

16:10 - 16:40 Tea

***Session 2: Catalysis (Chair: Steve Parker)***

16:40 G Hutchings: Catalysis using gold catalysts

17:00 A O’Malley: Molecular Mobility in Zeolites

17:20 T Chen: Hydrogen spillover mechanisms on metal supported material

17:40 N Harrison: Computational Characterisation of Heterogeneous Catalysts

18:00 M Sarwah: Atomistic Modelling: An Industrial Perspective

18:20 Close

19:30 Dinner (CH residents)

**Tuesday 11th April**

***Session 3: Facilities based science (Chair: Brian Fender)***

09:00 A Fitch: Powder diffraction studies on molecular materials

09:20 A Beale: Diffraction tomography of catalytic materials under reaction conditions

09:40 M Alfredsson: Pumping up the energy with XAS and calculations

10:00 K Harris: X-ray Birefringence Imaging: A New Synchrotron-Based Technique for Probing Molecular Orientational Distributions in Materials

10:20 S Matam: The role of in situ/operando spectroscopy in designing catalysts

10:40-11:10 Coffee

***Session 4: Minerals and Glasses (Chair: Avelino Corma)***

11:10 J Gale: Simulating the growth of minerals from water: Are we there yet?

11:30 E Hernandez: Thermodynamics of minerals from first principles

11:50 D di Tomasso: Atomistic Simulations of Water Confined in Hydroxyapatite Nanopores

12:10 A Cormack: Structure and Reactivity of Silicate Glasses

12:30 A Takada: Structural disorder and entropy in glass

12:50 – 14:00 Lunch (All)

***Session 5: Porous Solids (Chair: Joachim Sauer)***

14:00 G Sastre: Why bother analysing rings in zeolites?

14:20 L Gomez-Hortiguela: Computational studies of nanoporous zeolite-like aluminophosphate materials

14:40 R Ruiz Salvador: Automatic design of porous solids: opportunities for systematic research

15:00 R Grau-Crespo: Engineering the electronic excitation gap and band alignment of metal-organic frameworks

15:20 S Hamad-Gomez: Computational insights into the structure dynamics of porous materials

15:40-16:10 Tea

***Session 6: Computational and Materials Science (Chair: Sean Corish)***

16:10 F Cora: Computational studies of transition metal bearing solids

16:30 F Taylor: Modelling LaFeO3 for Intermediate Temperature SOFC Applications

16:50 A Shluger: Exciting oxides: one electron too many

17:10 X Zhang: Silicon Nonlinear Effect Assisted Magnetoresistance and Magnetic Logic

17:30 H Sithole: Advances in High Performance Computing in South Africa in support of Materials Science

17:50 L Whitmore: Web Tools for Protein Circular Dichroism Data

18:00 Close

19:00 Drinks reception

19:30 Conference dinner

**Wednesday 12th April**

***Session 7: Catalysis and Nanoscience (Chair: Nora de Leeuw)***

09:00 E Gibson: Developments in In Situ and Operando Spectroscopy by the Design Theme of the UK Catalysis Hub

09:20 C Cooper: Simulation of perovskite structure materials in catalysis

09:40 A Chutia: Catalytically important organic species on metal and metal oxide surfaces – a combined DFT and experimental study

10:00 S Bromley: From Nanoclusters to Nanostructured Solids: Insights and Predictions from Computational Modelling

10:20-10:50 Coffee

***Session 8: Materials and Surface Chemistry (Chair: Rob Jackson)***

10:50 A Rohl: Can Point Defects in Surfaces in Solution be Atomically Resolved by Atomic Force Microscopy?

11:10 D Arnold: Probing the mysterious phases of bismuth ferrite

11:30 S Parker: Modelling Interfaces for Energy and the Environment

11:50 R Jackson: From nuclear materials to nuclear clocks – some highlights of 36 years of materials modelling

12:10 R Catlow: Closing remarks

12:30 Close